

An alternative quantum fidelity for mixed states of qudits

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We give an alternative definition of quantum fidelity for two density operators on qudits in terms of the Hilbert-Schmidt inner product between them and their purity. It can be regarded as the well-defined operator fidelity for the two operators and satisfies all Jozsa's four axioms up to a normalization factor. One desire property is that it is not computationally demanding.

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Fidelity is an important concept in quantum information theory [1] and quantum chaos [2]. The well-known quantum fidelity for two general mixed states ρ_0 and ρ_1 is given by the Uhlmann's fidelity [3, 4, 5, 6]

$$\mathcal{F}(\rho_0, \rho_1) = \text{tr} \sqrt{\rho_0^{1/2} \rho_1 \rho_0^{1/2}}. \quad (1)$$

This fidelity has many nice properties such as concavity and multiplicativity under tensor product and it satisfies all Jozsa's four axioms [5]. However, it is not an easy task to make analytical evaluation of the fidelity and even numerical calculations due to the square roots of Hermitian matrix in the above equation. Quite recently, people tried to define new fidelities to avoid this difficulty. Miszczak et al. and Mendonça et al. defined the following fidelity [7, 8]

$$\mathcal{F}_1(\rho_0, \rho_1) = \text{tr}(\rho_0 \rho_1) + \sqrt{1 - \text{Tr}(\rho_0^2)} \sqrt{1 - \text{Tr}(\rho_1^2)}, \quad (2)$$

Another fidelity which is essentially is the same as \mathcal{F}_1 is defined by Chen et al. as [9]

$$\mathcal{F}_2(\rho_0, \rho_1) = \frac{1-r}{2} + \frac{1+r}{2} \mathcal{F}_1(\rho_0, \rho_1), \quad (3)$$

where $r = 1/(d-1)$ with d being the dimension of the Hilbert space. This fidelity displays a nice property that it has a clear hyperbolic geometric interpretation. Another property is that these two fidelities reduce to Uhlmann's fidelity in the special case of dimension $d = 2$.

One fundamental requirement for a definition of fidelity is that it must obey $F(\rho, \rho) = 1$. All the above three definitions satisfies this condition. However, it is not sufficiently emphasized in earlier studies that when two density matrix are orthogonal, the fidelity should be zero. This could be another fundamental requirement for

the fidelity. Consider the following density matrices

$$\begin{aligned} \rho_0 &= \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|), \\ \rho_1 &= \frac{1}{2}(|2\rangle\langle 2| + |3\rangle\langle 3|), \end{aligned} \quad (4)$$

acting on four-dimensional Hilbert space spanned by $\{|n\rangle, n = 0, 1, 2, 3\}$. Obviously, these two density matrix is orthogonal and the fidelity should be zero. After some simple calculations, we find that $\mathcal{F} = 0$, $\mathcal{F}_1 = 1/2$, and $\mathcal{F}_2 = 2/3$. Thus, in this strict sense it is appropriate to call \mathcal{F}_1 super-fidelity which acts as a useful upper bound for the Uhlmann's fidelity [7].

In this paper, we introduce an alternative fidelity defined, which satisfies Jozsa's axioms up to a normalization factor. And the fidelity is zero when two density matrices are orthogonal and is 1 when they are identical. We also discuss its other properties such as convexity and multiplicativity under tensor products.

The fidelity can be regarded as the operator fidelity [10] and thus we begin by introducing the definition of operator fidelity between two operators. Let \mathcal{H} be a d -dimensional Hilbert space. All linear operators on \mathcal{H} on its own is a d^2 -dimensional Hilbert space \mathcal{H}_{HS} . The inner product in this space is defined as the Hilbert-Schmidt product, i.e., for operators A and B , $\langle A|B \rangle = \text{Tr}(A^\dagger B)$. Thus, any linear operators on \mathcal{H} can be considered as a state on \mathcal{H}_{HS} . Thus, the fidelity of two states can be naturally be lifted to the operator level.

To define the operator fidelity between two operators A and B , we need to first normalize them as $A/\sqrt{\text{Tr}(AA^\dagger)}$ and $B/\sqrt{\text{Tr}(BB^\dagger)}$, respectively. Then, the operator fidelity is defined as

$$F(A, B) = \frac{|\text{Tr}(A^\dagger B)|}{\sqrt{\text{Tr}(AA^\dagger)\text{Tr}(BB^\dagger)}}. \quad (5)$$

If we consider two unitary operators U_0 and U_1 , the above fidelity reduces to

$$F(U_0, U_1) = \frac{1}{d} |\text{Tr}(U_0^\dagger U_1)|, \quad (6)$$

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which is studied in Ref. [10] and can be applied to measure the sensitivity of quantum systems to perturbations. If two density operator ρ and σ are considered, the operator fidelity reduces to

$$F(\rho_0, \rho_1) = \frac{|\text{Tr}(\rho_0 \rho_1)|}{\sqrt{\text{Tr}(\rho_0^2) \text{Tr}(\rho_1^2)}}. \quad (7)$$

This is a function of the Hilbert-Schmidt inner product and two purity (equivalent to linear entropy). The fidelity for two density operators can be considered as operator fidelity. On the other hand, it can also be regarded as fidelity between two states ρ_0 and ρ_1 . This is the alternative definition of the fidelity. One cannot simply define the fidelity as $|\text{Tr}(\rho_0 \rho_1)|$ as it becomes less than one when the two density matrices are identical, i.e., $\text{Tr}(\rho_0^2) < 1$.

It is easy to show that the fidelity F has the following desirable properties:

- (1) F is normalized. The maximum 1 is attained if and only if $\rho_0 = \rho_1$.
- (2) F is symmetric under swapping ρ_0 and ρ_1 , i.e., $F(\rho_0, \rho_1) = F(\rho_1, \rho_0)$.
- (3) The fidelity is invariant under unitary transformation U on the state space, i.e., $F(\rho_0, \rho_1) = F(U\rho_0 U^\dagger, U\rho_1 U^\dagger)$.
- (4) When one of the state is pure, say, $\rho_1 = |\psi\rangle\langle\psi|$, the fidelity reduces to $F(\rho_0, |\psi\rangle\langle\psi|) = \langle\psi|\rho_0|\psi\rangle/\text{Tr}(\rho_0^2)$.

To compare with Jozsa's four axioms, only the fourth property differs by a normalization factor $1/\text{Tr}(\rho_0^2)$. Then, we see that this fidelity satisfies all Jozsa's axioms up to a normalization factor [5]. Another obvious fact is that if two density matrices are orthogonal, the fidelity is zero. It is easy to check another nice property that the fidelity F is multiplicative under tensor products, i.e., $F(\rho_1 \otimes \rho_2, \sigma_1 \otimes \sigma_2) = F(\rho_1, \sigma_1)F(\rho_2, \sigma_2)$. The Uhlmann's fidelity also satisfies this property.

Next, we check that if F satisfies the property of concavity or convexity. By numerical calculations, we find that the following inequality

$$p_1 F(\rho_1, \sigma) + p_2 F(\rho_2, \sigma) \leq F(p_1 \rho_1 + p_2 \rho_2, \sigma), p_1, p_2 \geq 0$$

is satisfied for most matrices ρ_1, ρ_2 and σ for $p_1 + p_2 = 1$. However, the violation can also be found. The most simplest demonstration can be given if $\rho_1 = I/2$, $\rho_2 = |0\rangle\langle 0|$ and $\sigma = |1\rangle\langle 1|$ for $p_1, p_2 \in (0, 1)$. Here, states $|0\rangle$ and $|1\rangle$ are orthogonal and I is the 2×2 identity matrix.

To show the violation of concavity, let

$$\tilde{\rho} = p\rho_1 + (1-p)\rho_2 = (1-p/2)|0\rangle\langle 0| + p/2|1\rangle\langle 1|,$$

then

$$F(\tilde{\rho}, \sigma) = \frac{\langle 1|\tilde{\rho}|1\rangle}{\sqrt{\text{Tr}(\tilde{\rho}^2)}} = \frac{p}{\sqrt{2}[1 + (1-p)^2]^{1/2}},$$

and

$$pF(\rho_1, \sigma) + (1-p)F(\rho_2, \sigma) = pF(\rho_1, \sigma) = \frac{p}{\sqrt{2}}.$$

It is obvious that

$$F(\tilde{\rho}, \sigma) < pF(\rho_1, \sigma) + (1-p)F(\rho_2, \sigma)$$

for $p \in (0, 1)$.

That is to say, F satisfies neither concavity nor convexity. Since any measure is monotonically increasing (decreasing) if it is (i) unitarily invariant, (ii) jointly concave (convex) and (iii) invariant under the addition of an ancillary system [11], F is not monotonically increasing or decreasing under quantum operations.

As an application, we consider thermal equilibrium density matrix $\rho_k = \exp(-\beta H_k)/Z(\beta)$ ($k = 0, 1$) acting on d -dimensional Hilbert space [$Z_k(\beta) = \text{Tr}[\exp(-\beta H_k)]$ is the partition function for k -th system, $T = \beta^{-1}$ is the temperature, and the Boltzmann constant is assumed to be one]. From Eq. (7), the fidelity for the two thermal states is given by

$$\begin{aligned} F(\rho_0, \rho_1) &= \frac{\text{Tr}(e^{-\beta H_0} e^{-\beta H_1})}{\sqrt{\text{Tr}(e^{-2\beta H_0}) \text{Tr}(e^{-2\beta H_1})}} \\ &= \frac{\text{Tr}[(e^{-\beta H_0})^\dagger e^{-\beta H_1}]}{\sqrt{\text{Tr}[(e^{-\beta H_0})^\dagger e^{-\beta H_0}] \text{Tr}[(e^{-\beta H_1})^\dagger e^{-\beta H_1}]}}. \end{aligned} \quad (8)$$

It is well-known that imaginary time (or imaginary temperature) is essential in connecting quantum mechanics and statistical mechanics. If we make the Wick rotation, i.e., let $\beta = it$, the above equation reduces to

$$F(U_0, U_1) = 1/d |\text{Tr}(e^{itH_0} e^{-itH_1})|, \quad (9)$$

which is just the operator fidelity for two unitary operators U_k generated by Hamiltonian H_k . Thus, we see that the fidelity for two thermal states is connected to the operator fidelity for two unitary evolution operators by the Wick rotation by $\pi/2$. The fidelity introduced here is expected to be applicable to studies of phase transitions and quantum chaos.

In conclusion, we have introduced an alternative fidelity which satisfies Jozsa's four axioms up to a normalization factor. It has a desire property that is multiplicative under tensor products and undesire one that it is neither convex nor concave. The relations between this fidelity and the operator fidelity was clarified. Another merit is that it is not computationally demanding. From an measurement point of view, this fidelity is relatively easy to measure as it contains only the Hilbert-Schmidt inner product and two purity.

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